

Resonant Atom-Dimer Relaxation in Ultracold Atoms

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Three-body systems with large scattering length display universal phenomena associated with a discrete scaling symmetry. These phenomena include resonant enhancement of three-body loss rates when an Efimov three-body resonance is at the scattering threshold. In particular, there can be resonant peaks in the atom-dimer relaxation rate for large positive scattering length. We improve upon earlier studies and calculate the atom-dimer relaxation rate as a function of temperature using a Bose-Einstein distribution for the thermal average. As input, we use calculations of the atom-dimer scattering phase shifts from effective field theory.

Introduction: The Efimov effect is a phenomenon that occurs in a nonrelativistic 3-body system with resonant short-range interactions. Efimov discovered in 1970 that there are infinitely many 3-body bound states with an accumulation point at the scattering threshold when the S-wave scattering length a is tuned to the unitary limit $1/a = 0$ [1]:

$$E_T^{(n)} = (e^{-2\pi/s_0})^{n-n_*} \hbar^2 \kappa_*^2 / m, \quad (1)$$

where m is the mass of the particles, $s_0 \approx 1.00624$, and κ_* is the binding wavenumber of the branch of Efimov states labeled by n_* . The geometric spectrum in (1) is the signature of a discrete scaling symmetry with scaling factor $e^{\pi/s_0} \approx 22.7$. For a finite scattering length that is large compared to the range of the interaction, the universal properties persist but there will only be a finite number of Efimov states. The corrections to the unitary limit are calculable in perturbation theory [2, 3, 4]. The Efimov effect is just one example of universal phenomena in the 3-body system with large scattering length [5, 6]. For reviews of this “Efimov physics”, see Refs. [7, 8]. Here we focus on identical bosons in a single spin state and positive scattering length.

Since we are interested in applications to ultracold atoms, we refer to the bosons as atoms, their 2-body bound states as dimers, and their 3-body bound states as trimers. If the scattering length a is large and positive, there is a shallow dimer with binding energy $E_D = \hbar^2/(ma^2)$. Moreover, there is an infinite sequence of positive values of a for which there is an Efimov trimer at the atom-dimer scattering threshold [5]: $a = (e^{\pi/s_0})^n a_*$, where $a_* \approx 0.0708 \kappa_*^{-1}$ [9]. Another example of Efimov physics is an infinite sequence of positive values of a for which the 3-body recombination rate into the shallow dimer vanishes [10, 11, 12, 13]. The universal aspects of Efimov physics are determined by two parameters: the scattering length a and the Efimov parameter κ_* .

The alkali atoms used in most ultracold atom experiments have many deeply-bound diatomic molecules (deep dimers). Efimov physics is modified by the existence of the deep dimers because they provide inelastic channels

for scattering processes and the decay of trimers. If there is an Efimov trimer near the scattering threshold, there will be a resonant enhancement of inelastic scattering processes. When $a \approx (e^{\pi/s_0})^n a_*$, the resonant inelastic process is dimer relaxation, in which the collision of an atom and a shallow dimer produces an atom and a deep dimer [14]. If there are deep dimers, the universal phenomena associated with Efimov physics are determined by three parameters: a , κ_* , and a parameter η_* that determines the widths of Efimov trimers [14].

Experimental evidence for an Efimov trimer in ultracold Cs atoms was recently provided by their signature in three-body recombination rates [15]. This signature could be unravelled by varying the scattering length a over several orders of magnitude using a Feshbach resonance. More recently, possible evidence for an Efimov resonance was also obtained in atom-dimer scattering [16], in three-body recombination in a balanced mixture of atoms in three different hyperfine states of ^6Li [17, 18], and in a heteronuclear system of ^{41}K and ^{87}Rb [19].

In this paper, we focus on the Efimov resonance in atom-dimer scattering found in [16]. This process was previously considered in [14, 20]. We go beyond these earlier studies in various respects: we use the full effective field theory results for the atom-dimer phase shifts instead of the effective range expansion and perform a thermal average using the Bose-Einstein instead of the Boltzmann distribution. Moreover, we correct an error in the calculation of [20].

Atom-dimer scattering: We consider the scattering of an atom with mass $m_A = m$ and dimer with mass $m_D = 2m$. The wavenumbers \mathbf{p}_A and \mathbf{p}_D of the incoming atom and dimer, respectively, can be decomposed into the total wavenumber $\mathbf{p}_{\text{tot}} = \mathbf{p}_A + \mathbf{p}_D$ and the relative wavenumber $\mathbf{k} = \frac{2}{3}\mathbf{p}_A - \frac{1}{3}\mathbf{p}_D$. Because of Galilei invariance, the scattering observables depend on the relative wavenumbers and the collision energy E in the center-of-mass system only: $E = 3\hbar^2 k^2/(4m)$ where $k = |\mathbf{k}|$. The differential cross section for elastic atom-dimer scattering

is

$$\frac{d\sigma_{AD}^{(\text{elastic})}}{d\Omega} = |f_{AD}(k, \theta)|^2, \quad (2)$$

where $f_{AD}(k, \theta)$ is the scattering amplitude. The elastic cross section $\sigma_{AD}^{(\text{elastic})}$ is obtained by integrating Eq. (2) over the full solid angle. The total cross section (including elastic and inelastic contributions) can be calculated using the optical theorem:

$$\sigma_{AD}^{(\text{total})} = \frac{4\pi}{k} \text{Im} f_{AD}(k, \theta = 0), \quad (3)$$

such that the inelastic cross section is given by the difference of the total and elastic cross section. At low energies, higher partial waves with $L > 0$ are suppressed and the scattering amplitude is dominated by S-waves ($L = 0$):

$$f_{AD}(k) = [k \cot \delta_0^{AD}(k) - ik]^{-1}. \quad (4)$$

For the S-wave atom-dimer phase shift $k \cot \delta_0^{AD}(k)$, we will use the results from a calculation using the effective field theory of Ref. [21]. A convenient parametrization of these results was given in [7, 9]:

$$\begin{aligned} ka \cot \delta_0^{AD}(k) &= c_1(ka) \\ &+ c_2(ka) \cot[s_0 \ln(0.19 a/a_*) + \phi(ka)], \end{aligned} \quad (5)$$

where

$$\begin{aligned} c_1(ka) &= -0.22 + 0.39k^2a^2 - 0.17k^4a^4, \\ c_2(ka) &= 0.32 + 0.82k^2a^2 - 0.14k^4a^4, \\ \phi(ka) &= 2.64 - 0.83k^2a^2 + 0.23k^4a^4. \end{aligned} \quad (6)$$

This parametrization is valid up to the dimer breakup wavenumber of $k_D = 2/(\sqrt{3}a)$. A parametrization for higher wavenumbers beyond the dimer breakup exists [22] but will not be required for our purposes as we will demonstrate below.

To leading order in the large scattering length, atom-dimer relaxation can only proceed via S-waves. For the relaxation into deep dimers to take place, the atom and the dimer have to approach each other to very short distances. However, because of the angular momentum barrier this can only happen in the relative S-wave. The parametrization of the S-wave phase shift in Eqs. (5, 6) is therefore sufficient to calculate atom dimer-relaxation.

Atom-dimer relaxation: To incorporate the effects of deep dimers, we make the simple replacement in the amplitude [14]

$$\ln a_* \rightarrow \ln a_* - i\eta_*/s_0, \quad (7)$$

where η_* determines the probability for an atom and a dimer to scatter into an energetic atom and deep dimer pair at short distances. This inelastic process generates the width of the Efimov resonances. The phase shift becomes imaginary even below the dimer breakup threshold

and the released binding energy is converted to the kinetic energy of the recoiling atom and dimer. They thus are lost to the system. The event rate β for this dimer relaxation process in an ultracold gas of atoms and dimers can be written as

$$\frac{d}{dt}n_A = \frac{d}{dt}n_D = -\beta n_A n_D, \quad (8)$$

where n_A and n_D denote the number density of the atoms and dimers, respectively.

For an ensemble of atoms and dimers at nonzero temperature that are held in a trap, temperature and trap geometry have to be included in the calculation of the observed dimer losses. The dimer loss rate can be expressed as

$$\frac{d}{dt}N_D = - \int d^3r \prod_{i=A,D} \left[\int \frac{d^3p_i}{(2\pi)^3} n_i(p_i, r) \right] g(k), \quad (9)$$

where N_D is the number of dimers and we use the generalized Bose-Einstein distribution function

$$n_i(p_i, r) = \left[\exp \left\{ \left(\frac{\hbar^2 p_i^2}{2m_i} + \frac{m_i \bar{\omega}^2 r^2}{2} - \mu_i \right) / k_B T \right\} - 1 \right]^{-1} \quad (10)$$

with $i = A, D$ denoting an atom or dimer, respectively. The properties of the trap enter via the average trap frequency $\bar{\omega}$ while the function $g(k)$ to be averaged is given by

$$\begin{aligned} g(k) &= \frac{3\hbar k}{2m} \sigma_{AD}^{(\text{inel.})}(k) \\ &= \frac{3\hbar k}{2m} \left(\sigma_{AD}^{(\text{total})}(k) - \sigma_{AD}^{(\text{elastic})}(k) \right). \end{aligned} \quad (11)$$

In the limit $k \rightarrow 0$, $g(k)$ reduces to the relaxation rate constant at zero temperature. Note that the function $g(k)$ introduces an implicit dependence on the angle between \mathbf{p}_A and \mathbf{p}_D . The chemical potentials μ_i are fixed via the equation

$$\int d^3r \int \frac{d^3p_i}{(2\pi)^3} n_i(p_i, r) = N_i, \quad (12)$$

with N_i being the particle number and $i = A, D$.

All angular integrations except for one can be carried out immediately and the expression (9) can be rewritten as:

$$\begin{aligned} \frac{d}{dt}N_D &= -\frac{1}{2\pi^3} \int_0^\infty r^2 dr \int_0^\infty p_{tot}^2 dp_{tot} \int_0^\infty k^2 dk \\ &\times \int_{-1}^1 dx n_A(p_A, r) n_D(p_D, r) g(k), \end{aligned} \quad (13)$$

where x is the cosine of the angle between \mathbf{p}_{tot} and \mathbf{k} .

In evaluating Eq. (13), we will cut off the integral over k at the breakup wavenumber $k_D = 2/(\sqrt{3}a)$ since the parametrization in Eqs. (5, 6) is only valid up to k_D . We have estimated the error from this simplification by using

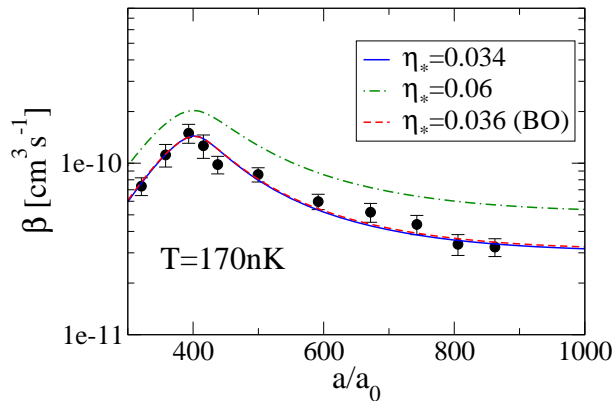


FIG. 1: The dimer relaxation coefficient β as a function of a/a_0 for $T = 170$ nK, $a_* = 397a_0$, and different values of η_* . The data points are from [16]. BO indicates a Boltzmann average.

the unitary bound i/k for the S-wave scattering amplitude $f_{AD}(k)$. For the data of Ref. [16], the error involved is largest for the largest scattering length considered but even there only adds up to 0.2% for the largest temperature $T = 170$ nK. As a consequence, we can simply neglect the contribution from $k > k_D$ in the analysis of the data.

Results and Discussion: We now apply our formalism to the experimental data for the atom-dimer relaxation rate of ultracold Cs atoms as a function of the scattering length obtained by Knoop et al. [16]. Our free parameters are a_* which determines the position of the resonance and η_* which determines its width. These parameters cannot be calculated in our approach and must be taken from experiment. We will determine a_* and η_* from the data of Knoop et al. and compare our results with what is known from other experiments. In Ref. [16], the dimer relaxation coefficient was extracted from the dimer loss data using a loss model resulting in the rate equation

$$\frac{d}{dt}N_D = -\frac{8}{\sqrt{27}}\beta\bar{n}_AN_D + \text{dimer loss term}, \quad (14)$$

with $\bar{n}_A = [m\bar{\omega}^2/(4\pi k_B T)]^{3/2}N_A$ the mean atomic density. In order to compare our calculation with the experiment of Knoop et al., we extract a value for β from our result for dN_D/dt (cf. Eq. (13)) using

$$\beta \equiv -\frac{\sqrt{27}}{8\bar{n}_AN_D}\frac{d}{dt}N_D. \quad (15)$$

We start with the data at $T = 170$ nK and fix the chemical potentials as described above. For atom number $N_A = 10^5$, dimer number $N_D = 4 \times 10^3$, and an average trap frequency of $\bar{\omega} = 45$ Hz [23], we obtain the chemical potentials $\mu_A = -2.74 \times 10^{-7} k_B K$ and $\mu_D = -8.17 \times 10^{-7} k_B K$. In Fig. 1 the data for the recombination constant β is shown together with our best

fit as the solid (blue) line. We only take into account data points for $a > 300a_0$. This fit yields $\chi^2/dof = 1.2$. We obtain for the peak position $a_* = 397a_0$ and for the resonance width parameter $\eta_* = 0.034$. Also shown as a dashed-dotted (green) line is the resulting curve for the same resonance position but with $\eta_* = 0.06$. This value of η_* was obtained from fitting the three-body recombination resonance in Cs for negative scattering length in [15]. It is also compatible with the three-body recombination data for positive scattering length presented in the same paper.¹ However, the data for $a > 0$ are not very sensitive to the precise value of η_* and values of η_* as small as 0.01 would also be compatible. The width parameter η_* should only be weakly dependent on the magnetic field in a universal region [7]. In first approximation it can be assumed to remain constant. A more serious puzzle is that the resonance position $a_* = 397a_0$ extracted from the dimer relaxation data is not compatible with the value $a_* \approx 1200a_0$ found in [15]. The three-body recombination data cannot be satisfactorily described using $a_* = 397a_0$. This disagreement requires further study. However, one has to keep in mind that the atom-dimer resonance is at the border of the universal region since the van der Waals length scale is $l_{vdW} \approx 200a_0$ for Cs atoms.

For temperatures much larger than the Bose-Einstein condensation temperature, the thermal average can be replaced by a Boltzmann average. The critical temperatures are estimated by setting the chemical potential to zero and solving Eq. (12) for the critical temperature. This yields $T_{c,A} \approx 94$ nK for the atoms and $T_{c,D} \approx 32$ nK for the dimers. Therefore, it seems justified to use Boltzmann distributions instead of the Bose-Einstein distribution functions n_i . The resulting calculation for β is analogous to the method of Ref. [20] but uses the parametrization of the scattering phase (5) instead of an effective range expansion. The resulting curve is also shown in Fig. 1 as the dashed (red) line. We remark that in the numerical evaluation of Eq. (8) in Ref. [20] a factor of k^2 in the thermal average was omitted. This led to a wrong normalization of the curves in Figs. 1 and 2 of this reference. The dashed line obviously also describes the data quite well but yields $\eta_* = 0.036$. This shows how temperature dependence and averaging methods can partly be compensated by adjusting the width parameter η_* . For an accurate determination of η_* , reliable temperature and particle number measurements are thus crucial.

Using the effective range expansion for the atom-dimer scattering amplitude as in Ref. [20] instead of the phase shift parametrization of Eqs. (5, 6) does not alter the overall shape or normalization of the dimer relaxation coefficient β . However, the extracted value of

¹ Note that in the Cs experiment of [15] the regions $a > 0$ and $a < 0$ are not required to have the same parameters since they are separated by a zero in the scattering length rather than a pole. See also the discussion in [16].

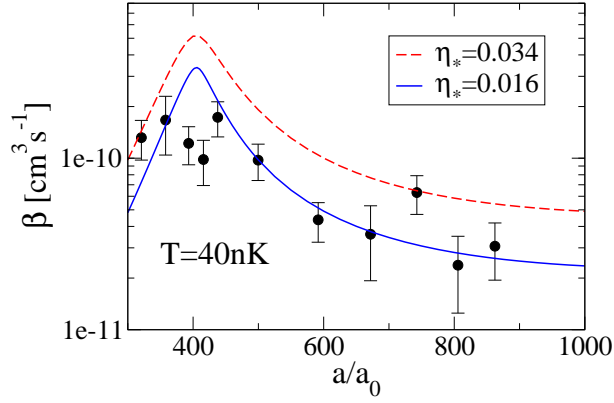


FIG. 2: The dimer relaxation coefficient β as a function of a/a_0 for $T = 40$ nK, $a_* = 397a_0$, and different values of η_* . The data points are from [16].

a_* is shifted by about 3% to a higher value whereas η_* remains unchanged. The scattering length approximation with the atom-dimer scattering length given by $a_{AD}/a = 1.46 + 2.15 \cot[s_0 \ln(a/a_*) + i\eta_*]$ does not lead to an equally good fit result. The obtained values for β are smaller especially for higher values of a . Besides a change in peak position, width and height, we can only obtain a χ^2/dof of 3 – 4.

We now turn to the data for $T = 40$ nK [16] and compare them to our theoretical results for different values of η_* . Here, the atom and dimer numbers are $N_A = 3 \times 10^4$ and $N_D = 4 \times 10^3$, and the trap frequency is $\bar{\omega} = 25.2$ Hz [16] leading to the chemical potentials $\mu_A = -1.21 \times 10^{-8} k_B K$ and $\mu_D = -8.87 \times 10^{-8} k_B K$. The critical temperatures are estimated as $T_{c,A} \approx 35$ nK for the atoms and $T_{c,D} \approx 18$ nK for the dimers such that the temperature is only slightly larger than the critical temperature for the atoms. In Fig. 2 we show the data for the relaxation coefficient β at $T = 40$ nK together with our fit results. The dashed (red) line gives our prediction for the relaxation coefficient β using the parameters obtained by fitting the 170 nK data. The prediction is about a factor 2 too large compared to the data. The

dip in the data at the peak position represented by the third and fourth data point cannot be reproduced within our theory. If it is not simply a statistical fluctuation, it must be due to physics not captured in our theory such as non-universal effects or four-body physics [24, 25, 26]. If we keep the resonance position at $a_* = 397a_0$ but fit the parameter η_* to the 40 nK data excluding the third and fourth data point, we obtain the solid (blue) line. Still excluding the third and fourth data point this gives $\eta_* = 0.016$ with $\chi^2/dof = 1.5$ and describes the data satisfactorily.

In summary, we have calculated the atom-dimer relaxation rate for large positive scattering length in a universal zero-range approach. We have improved on previous studies [14, 20] by using a Bose-Einstein distribution for the thermal average and calculations of the atom-dimer scattering phase shifts from effective field theory. Our results were then applied to the atom-dimer relaxation data for Cs obtained by Knoop et al. [16]. Fitting the resonance position and width parameters a_* and η_* , we could get a good description of the 170 nK data. Using these parameters, we overpredict the relaxation data at 40 nK by a factor of two. Moreover, our theory is not able to reproduce the dip in the 40 nK data directly at the resonance position and the corresponding physics appears to be missing in our theory. We demonstrated that this discrepancy is neither due to the thermal averaging procedure nor due to the phase shift parametrization used. The resonance position at the border of the universal region and the mismatch in the extracted resonance position from atom-dimer relaxation and the three-body recombination data [15] suggests that non-universal physics could be responsible. However, it is also conceivable that four-body losses become important at the lower temperature. This question deserves further study.

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